



Karsili, T. N. V., Marchetti, B., & Ashfold, M. N. R. (2016). Mechanistic Insights into Excited State Intramolecular Proton Transfer in Isolated and Metal Chelated Supramolecular Chemosensors. *Dalton Transactions*, 45, 18921-18930. <https://doi.org/10.1039/C6DT03906E>

Publisher's PDF, also known as Version of record

License (if available):
CC BY

Link to published version (if available):
[10.1039/C6DT03906E](https://doi.org/10.1039/C6DT03906E)

[Link to publication record in Explore Bristol Research](#)
PDF-document

This is the final published version of the article (version of record). It first appeared online via Royal Society of Chemistry at <https://doi.org/10.1039/c6dt03906e> . Please refer to any applicable terms of use of the publisher.

University of Bristol - Explore Bristol Research

General rights

This document is made available in accordance with publisher policies. Please cite only the published version using the reference above. Full terms of use are available:
<http://www.bristol.ac.uk/red/research-policy/pure/user-guides/ebr-terms/>

Electronic supplementary information for:

**Mechanistic Insights into Excited State Intramolecular Proton Transfer in
Isolated and Metal Chelated Supramolecular Biosensors.**

Tolga N. V. Karsili^{a,b*}, Barbara Marchetti^{a,b} and Michael N. R. Ashfold^b

^a*Department of Chemistry, Technische Universität München, Lichtenbergstrasse 4, 85748, Garching
Germany.*

^b*School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom.*

Figure S1: Minimum energy geometries and dominant orbital excitation accompanying the lowest three singlet electronic transitions of Cd^{2+} –HDBO' (right) and Hg^{2+} –HDBO' (left).

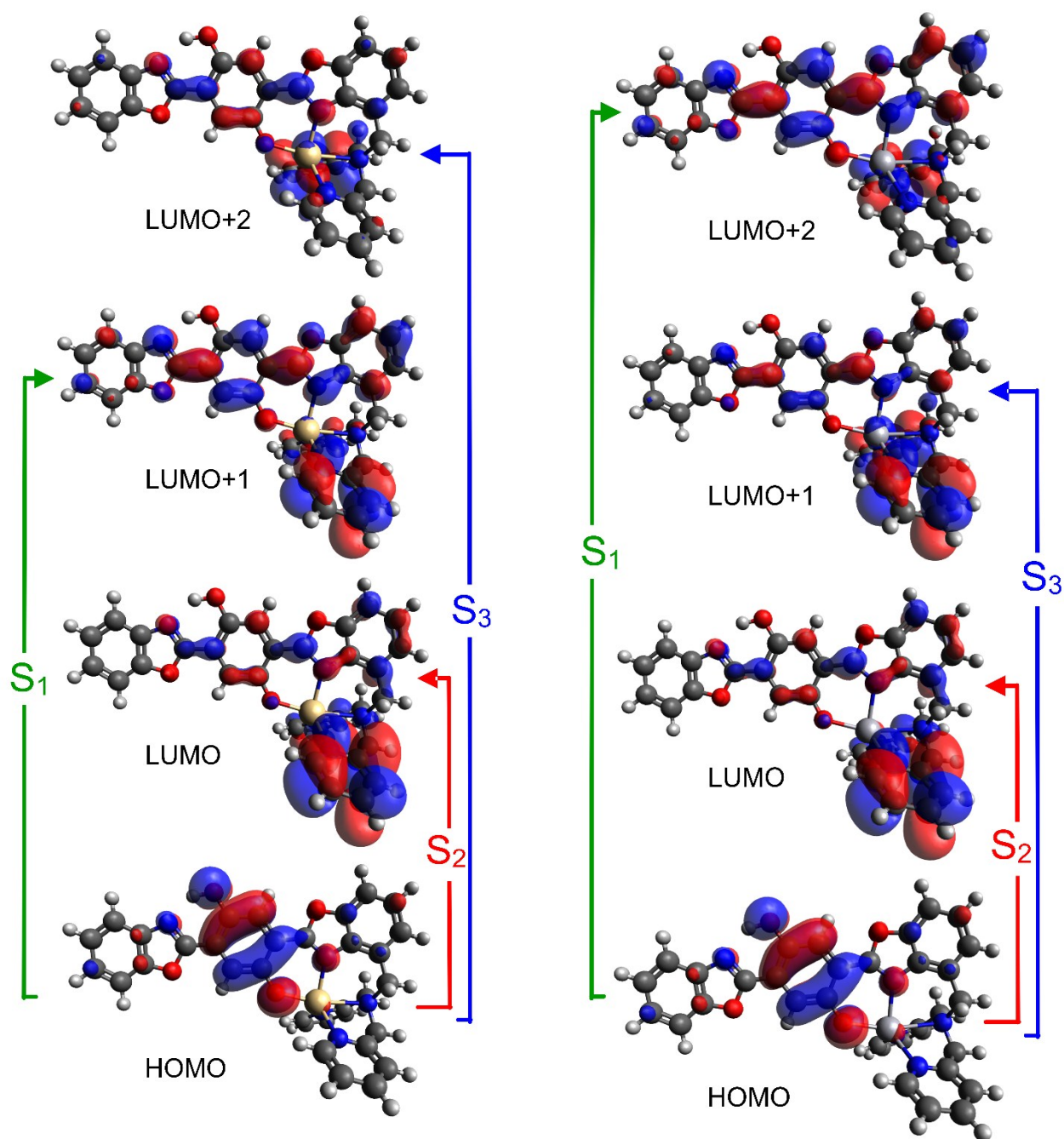


Figure S2: Magnitude and direction of the permanent dipole moment of HBO at the minimum energy geometries of (a) the S_0 state, (b) the S_1 *enol* conformer and (c) the S_1 *keto* minimum at planar geometries.

